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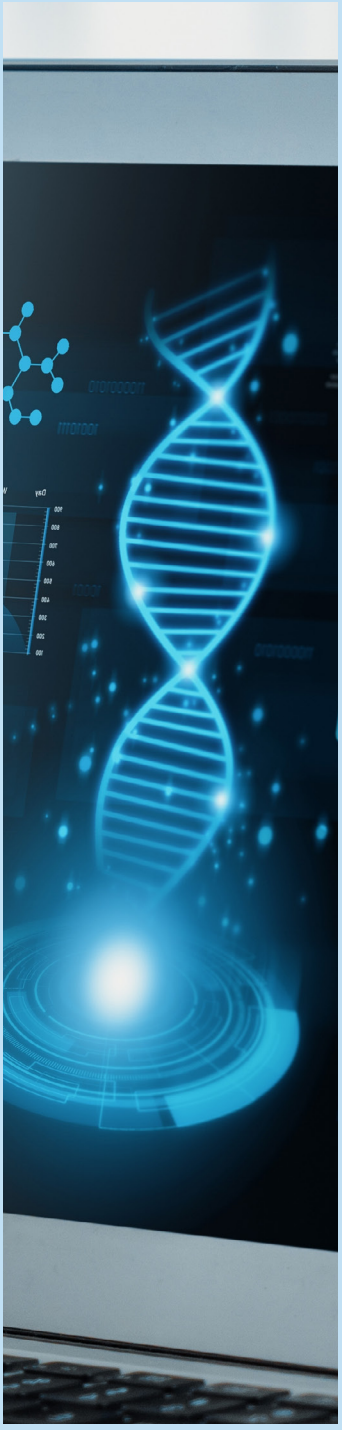

ACCELERATING DRUG DISCOVERY WITH AI – A STRATEGIC ROADMAP

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1. Executive Summary

The pharmaceutical industry faces mounting pressure to accelerate drug discovery while reducing costs and failure rates. Traditional methods take **12-15 years** and cost over **$2.6 billion per drug**, with a **90% failure rate in clinical trials**. Artificial Intelligence (AI) is emerging as a game-changer, significantly improving **target identification, lead discovery, clinical trial execution, and post-market surveillance.**

2. How AI is Transforming Drug Discovery

AI's impact spans **every stage** of the drug development lifecycle. Below is a **stage-wise breakdown** of how AI is reshaping the industry:

A) Target Identification & Validation

Challenges: Identifying disease-relevant targets from vast genomic and proteomic data.

AI Solutions:

Machine Learning for Data Mining:

Identifies correlations in disease pathways (e.g., BRCA mutations in breast cancer).

Deep Learning for Structural Biology:

Tools like **AlphaFold** predict protein structures with high accuracy.

Knowledge Graphs & NLP:

AI connects scientific literature, clinical data, and research findings to uncover novel targets.

B) Hit Identification & Lead Optimization

Challenges: Screening millions of compounds is slow and costly.

AI Solutions:

Virtual Screening:

AI models predict the best drug candidates faster than traditional high-throughput screening.

Generative AI for Drug Design:

GANs and VAEs generate novel molecules with desired properties.

Predictive Models for Drug Properties:

AI optimizes bioavailability, solubility, and toxicity.

C) Preclinical Testing

Challenges: Predicting safety and efficacy before human trials.

AI Solutions:

AI for Toxicity Prediction:

Models like **DeepTox** assess toxicity early.

Simulations via Quantitative Systems Pharmacology (QSP):

AI models predict drug interactions in the human body.

Robotic Automation:

AI-driven labs speed up preclinical experimentation.

D) Clinical Trials & Patient Stratification

Challenges: Recruiting the right patients and reducing trial failures.

AI Solutions:

AI for Patient Selection:

AI identifies high-response patient subgroups, improving trial success rates.

Virtual Clinical Trials:

AI-powered simulations reduce reliance on large-scale trials.

Adaptive Trial Design:

AI adjusts trial parameters in real-time based on evolving data.

E) Post-Market Surveillance & Drug Safety

Challenges: Monitoring real-world safety and efficacy.

AI Solutions:

AI-driven Pharmacovigilance

AI scans patient records and social media for adverse event signals.

Pattern Recognition for Side Effects

Machine learning identifies rare adverse reactions.

3. "PAIVC Framework – The Business Playbook for AI in Drug Discovery

To **strategically implement AI**, we propose the **PAIVC framework**, which outlines the **five core pillars:**

Pillar	Description	AI-Driven Methods Used
Predictive Target Discovery	AI identifies and validates disease targets faster.	Data Mining, Knowledge Graphs, AlphaFold
AI-Augmented Lead Discovery	AI optimizes hit identification and lead selection.	Virtual Screening, Generative AI, Predictive Modeling
Intelligent Preclinical Testing	AI reduces risks and improves safety predictions.	DeepTox, QSP Models, Robotic Experimentation
Virtualized Clinical Execution	AI enhances patient stratification and trial design.	AI-Driven Patient Selection, Virtual Trials, Adaptive Design
Continuous AI-Powered Safety	AI ensures long-term drug safety post-approval.	Pharmacovigilance, Adverse Event Detection

Why PAIVC Matters:

a) Provides a **structured roadmap** for AI adoption in life sciences.

b) Maps AI solutions directly to **business impact and ROI.**

c) Ensures **faster time-to-market** and **cost efficiency.**

Table 1: AI driven Drug discovery Time to Market

Drug Discovery Process	Traditional Timeline (Years)	AI-Driven Timeline (Years)	Reduction (%)	Total Reduction (Years) for 250 drugs
Target Identification	1-2	0.5-1	50%	250-500 years
Lead Compound Discovery	2-3	0.5-0.75	66-75%	375-562.5 years
Preclinical Development	3-4	1-2	50-66%	250-500 years
Clinical Trials	6-8	3-4	50%	750-1000 years
Total Time to Market	**10-15**	**4-6**	**60-66%**	**1525-2562.5 years**

4. Reinventing Life Sciences in the age of AI/Gen AI:

Infosys has emerged as a key player in leveraging these technologies to address critical challenges in drug discovery and development. Below are two groundbreaking use cases

Case Study 1: Infosys AI/ML-Based Drug Repurposing Solution

Description:

Infosys's Drug Repurposing Platform empowers pharmaceutical companies to identify new indications for existing drugs. Its cloud-native, microservices architecture ensures **scalability and accessibility.**

Solution Details:

In-Silico Modelling:

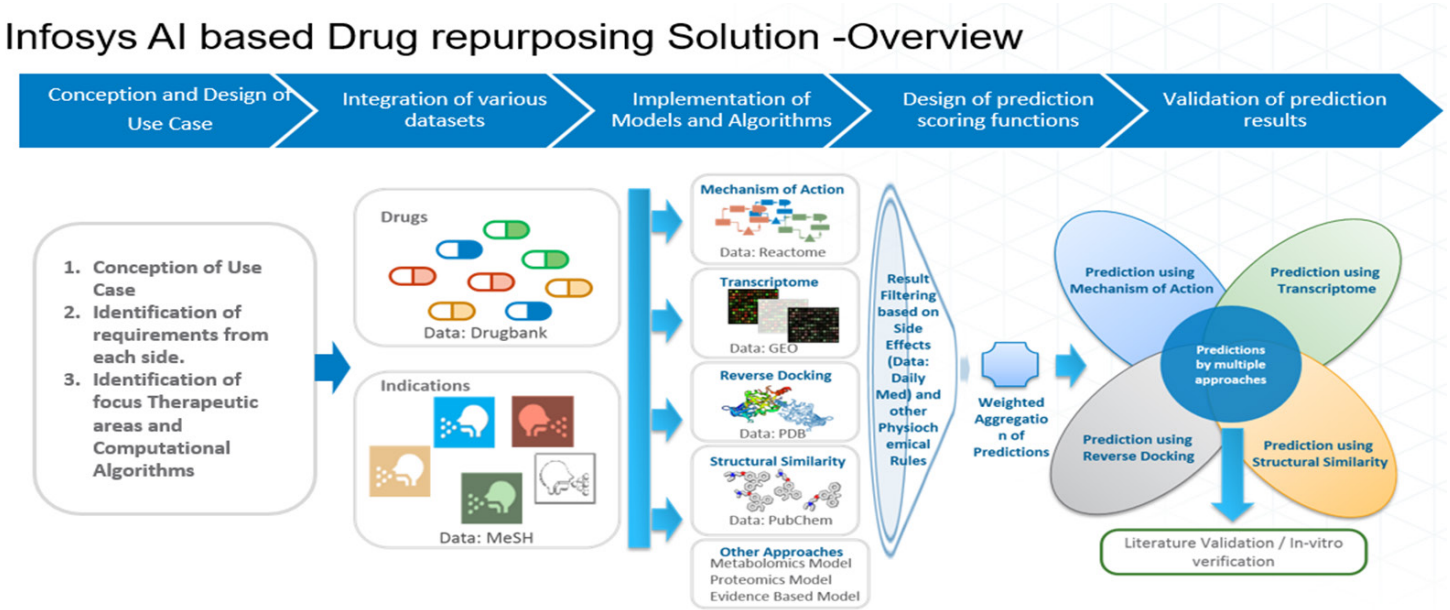
A computational approach that simulates biological processes—to identify potential new uses for existing drugs. For example, the platform uses advanced algorithms to analyse molecular structures and predict how they might interact with different disease pathways, accelerating hypothesis generation and validation. This approach significantly reduces the time and cost associated with developing new molecules or conducting safety studies, depending on the drug's development stage.

Integrated Data and Algorithms:

By combining public and proprietary datasets with algorithms for Mechanism of Action (MoA), which explains how a drug produces its effects, Transcriptome analysis (studying RNA expression levels), Reverse Docking (predicting potential targets for a drug), and Compound Structure evaluation, the platform generates unique and actionable insights.

Patent Innovation:

Infosys's solution is protected under **Patent # US 20150227700A1,** highlighting its proprietary **"Mechanism of Action" methodology.**



Case Study 2: Infosys Ligand Identification and Matching Tool

Description:

The Ligand Identification and Matching Tool identifies molecules, known as ligands, that can bind to specific active sites on proteins. Ligands are small molecules that interact with proteins to influence their function, while active sites are the regions on a protein where these interactions occur, often critical to the disease process. By creating detailed profiles of ligands, this system enables targeted and efficient drug discovery.

Solution Details:

Annotated Ligand Profiles:

Using structural and binding data from input ligands, the tool generates comprehensive profiles by analyzing chemical and stereochemical properties.

Advanced Search Algorithms:

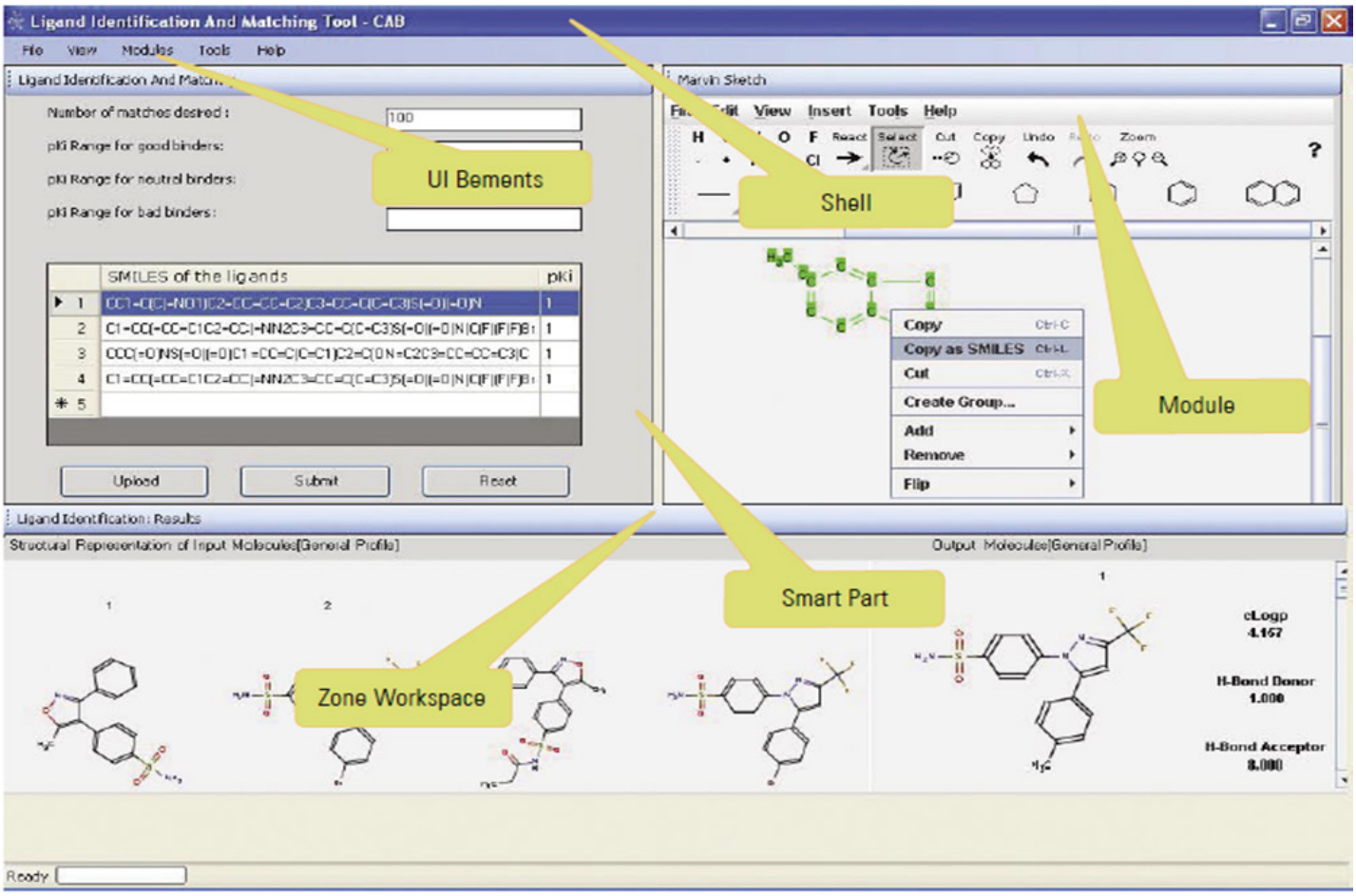
The system searches annotated molecular databases to identify additional ligands that can bind to the same protein target, scoring them using substitution matrix datasets.

User-Friendly Interface:

Researchers access input ligands, identified ligands, and related literature through an intuitive interface, enhancing usability.

Patent Innovation:

Infosys's solution is protected under Patent # US8468001B2, highlighting its proprietary "Ligand identification and matching software tools".



5. Conclusion

AI is **not just a technology upgrade—it's a paradigm shift in drug discovery.** The **PAIVC framework** provides a clear roadmap for AI adoption, ensuring that pharmaceutical companies stay ahead in an increasingly competitive industry. By embracing AI for **target identification, drug design, clinical trials, and safety monitoring,** organizations can bring life-saving drugs to patients faster and more cost-effectively.

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About the Authors

Jayadhar Gundu

(Consultant) at IC-LS

Jayadhar Gundu bringing a unique blend of business acumen and technical expertise drawn from over 7 years of experience across diverse sectors. With a robust background in life sciences consulting and the manufacturing domain, he has delivered transformative solutions in supply chain management. His proficiency in process improvement has led to significant operational gains and enhanced performance for clients. As a responsible AI practitioner he is committed to ethical AI deployment, ensuring that AI technologies are used responsibly and effectively to benefit the life sciences industry.

Sapna Bhardwaj

(Consultant) IC LS

Sapna is a seasoned life sciences consultant with over nine years of experience in R&D, Project and Quality Management, Data Analysis, and Computer System Validation (CSV). She has successfully led projects in safety and quality, driving continuous process improvements to enhance client performance. Passionate about innovation, she is eager to explore AI technologies and their responsible application in the life sciences industry.

For more information, contact askus@infosys.com

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